

Three-Qubit Gate Realization Using Single Quantum Particle

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Abstract

Using virtual spin formalism it is shown that a quantum particle with eight energy levels can store three qubits. The formalism allows to realize a universal set of quantum gates. Feasible formalism implementation is suggested which uses nuclear spin-7/2 as a storage medium and radio frequency pulses as the gates. One pulse realization of all universal gates has been found, including three-qubit Toffoli gate.

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1 Introduction

Toffoli proved [1] that a classical reversible computer can be constructed using a universal three-bit gate CCNOT (“controlled controlled NOT” or “double controlled NOT”). Deutsch has shown that in quantum information theory the generalized CCNOT gate - CCUT gate (“controlled controlled unitary transformation” or “double controlled unitary transformation”) [2] - also is a universal one. However to realize CCUT is not an easy task since there is no three body interaction in Nature. A way round was found Barenco *et al.* [3]: it was proved that CCUT can be realized using five two qubit CUT (“controlled unitary transformation”) gates. Such an approach was used in the NMR implementation of Toffoli gate [4, Eq. (38) and (39)].

The virtual spin formalism developed in [5] is used in the present paper to physically implement CCUT in a simplest possible way - using one pulse and one quantum particle.

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2 The quantum information notation for gates of system of three real spins-1/2

In quantum information the gates for the three real spins-1/2 system usually are written in Hilbert space Γ which is a direct product $\Gamma = \Gamma_Q \otimes \Gamma_R \otimes \Gamma_S$ of the Hilbert spaces of three real spins-1/2 Q, R, S . As a basis of Γ the following eight functions can be chosen which will be used later

$$\begin{aligned} |0\rangle &= |000\rangle, & |1\rangle &= |001\rangle, & |2\rangle &= |010\rangle, & |3\rangle &= |011\rangle, \\ |4\rangle &= |100\rangle, & |5\rangle &= |101\rangle, & |6\rangle &= |110\rangle, & |7\rangle &= |111\rangle, \end{aligned} \quad (1)$$

where $|M\rangle = |m_Q, m_R, m_S\rangle$, for example, $|5\rangle = |m_Q = +1/2, m_R = -1/2, m_S = +1/2\rangle$ and so on.

Let us consider all possible gates with NOT operation. In three spin system there are three NOT gates - the gate, which invert one spin leaving two others unchanged,

$$\begin{aligned} NOT_Q &= |1m_R m_S\rangle \langle 0m_R m_S| + |0m_R m_S\rangle \langle 1m_R m_S|, \\ NOT_R &= |m_Q 1m_S\rangle \langle m_Q 0m_S| + |m_Q 0m_S\rangle \langle m_Q 1m_S|, \\ NOT_S &= |m_Q m_R 1\rangle \langle m_Q m_R 0| + |m_Q m_R 0\rangle \langle m_Q m_R 1|. \end{aligned} \quad (2)$$

There are six CNOT gates. For example, when “master” spin R state controls “slave” spin Q state leaving spin S state unchanged

$$\begin{aligned} CNOT_{R \rightarrow Q} &= |00m_S\rangle \langle 00m_S| + |11m_S\rangle \langle 01m_S| + \\ &|10m_S\rangle \langle 10m_S| + |01m_S\rangle \langle 11m_S|. \end{aligned} \quad (3)$$

Reverse gate

$$\begin{aligned} CNOT_{Q \rightarrow R} &= |00m_S\rangle \langle 00m_S| + |01m_S\rangle \langle 01m_S| + \\ &|11m_S\rangle \langle 10m_S| + |10m_S\rangle \langle 11m_S|. \end{aligned} \quad (4)$$

Other four CNOT gates can be written for pairs RS and QS by analogy.

There are three CCNOT gates. For example, when two “master” spins Q and R control one “slave” S one has

$$\begin{aligned} CCNOT_{Q,R \rightarrow S} &= |000\rangle \langle 000| + |001\rangle \langle 001| + \\ &|010\rangle \langle 010| + |011\rangle \langle 011| + \\ &|100\rangle \langle 100| + |101\rangle \langle 101| + \\ &|111\rangle \langle 110| + |110\rangle \langle 111|. \end{aligned} \quad (5)$$

The gates $CCNOT_{R,S \rightarrow Q}$ and $CCNOT_{S,Q \rightarrow R}$ can be written by analogy.

3 Virtual spin formalism

In the realized NMR quantum gates one qubit NOT operation is implemented as a spin rotation under influence of a resonant pulse. Whereas conditional quantum dynamics, which is necessary for two qubit CNOT gate, is implemented using system with two body spin-spin interaction [4].

It will be shown later in this paper that conditional quantum dynamics can be realized on one spin-7/2 without using spin-spin interactions. Another specific feature of such an approach is that all three types of gates NOT, CNOT and CCNOT can be implemented using just one RF pulse. These advantages are possible due to special information coding onto spin-7/2 states - this coding was introduced in [5] under the name virtual spin formalism.

The main idea of the virtual spin formalism can be expressed as follows. As a basis for the spin-7/2 Hilbert space $\Gamma_{7/2}$ the eigen functions $|\chi_m\rangle$ of I_z operator ($m = \pm\frac{1}{2}, \pm\frac{3}{2}, \pm\frac{5}{2}, \pm\frac{7}{2}$) or eigen functions $|\psi_m\rangle$ of total spin energy operator (defined below) can be chosen. Let us instead

$$m = -\frac{7}{2}, -\frac{5}{2}, -\frac{3}{2}, -\frac{1}{2}, +\frac{1}{2}, +\frac{3}{2}, +\frac{5}{2}, +\frac{7}{2}$$

use notation $M = 0, 1, 2, 3, 4, 5, 6, 7$ and therefore instead $|\psi_m\rangle$ to use $|\psi_M\rangle$. Then formally $|\psi_M\rangle$ can be mapped to $|M\rangle = |m_Q, m_R, m_S\rangle$ which is a state of virtual spins-1/2 Q, R, S . Then in order to implement all above mentioned gates it is necessary to find such external influence on real spin-7/2, which would have in the basis $|\psi_M\rangle$ the evolution propagator matrices of the same operational forms as the above written gates in the basis $|M\rangle$.

4 Spin-7/2 system and physical realization of gates

Let us consider the system of nuclear spin $I = 7/2$ placed in constant magnetic field H_0 and axially symmetrical electric crystal field:

$$\begin{aligned} \mathcal{H} &= \mathcal{H}_z + \mathcal{H}_Q, \\ \mathcal{H}_z &= -\hbar\omega_0 I_z, & \mathcal{H}_Q &= \frac{1}{2}\hbar\omega_Q \sum_{\alpha=0,\pm 1,\pm 2} Q_\alpha q_{-\alpha}, \\ Q_0 &= I_z^2 - \frac{1}{3}I(I+1), & q_0 &= 3\cos^2\theta - 1, \\ Q_{\pm 1} &= I_z I_{\pm 1} + I_{\pm 1} I_z, & q_{\pm 1} &= \sin\theta \cos\theta e^{\pm i\phi}, \\ Q_{\pm 2} &= I_{\pm 1}^2, & q_{\pm 2} &= \frac{1}{2}\sin 2\theta e^{\pm i2\phi}, \\ \omega_Q &= \frac{3eqQ}{[2I(2I-1)\hbar]}, & I_{\pm 1} &= I_x \pm iI_y, \end{aligned} \tag{6}$$

where e - the electron charge, Q - nuclear quadrupole moment, $I_\beta (\beta = x, y, z)$ - spin components, $2eq$ - the electric field gradient value, θ and ϕ - the polar angles, which define its axes orientation in laboratory system frame. Let us consider

a case when $\omega_Q \ll \omega_0$ so quadrupole interaction influence can be calculated using perturbation theory. It is supposed that quadrupole interaction much greater than the spin resonance line width, so the spectrum consists of seven well separated resonance lines.

The first approximation gives the following energy levels and eigen functions:

$$\begin{aligned} E_m &\equiv \hbar \varepsilon_m = -\hbar \omega_0 m + \hbar \omega_Q q_0 (m^2 - \frac{21}{4}), \\ |\psi_m\rangle &= \chi_m + \sum_{m \neq k} \frac{\langle \chi_k | \mathcal{H}_Q | \chi_m \rangle}{\hbar \omega_0 (k - m)} \chi_k, \end{aligned} \quad (7)$$

here the normalization factor of $|\psi_m\rangle$ is omitted.

For simplicity the projective operators P_{mn} notation will be used. They are matrices 8×8 with all elements p_{kl} equal zero except one $p_{mn} = 1$. They have very simple relations:

$$P_{kl} P_{mn} = \delta_{lm} P_{kn}, P_{mn} = P_{nm}^+, P_{mn} |\psi_k\rangle = \delta_{nk} |\psi_m\rangle. \quad (8)$$

An RF pulse, which is resonant for energy levels E_m and E_n ($E_m > E_n$), results in evolution operator [5]

$$\begin{aligned} V_X(\phi_{mn}, f) &= \hat{1} + (P_{nn} + P_{mm})(\cos \frac{1}{2} \phi_{mn} - 1) + \\ &\quad i(P_{mn} e^{if} + P_{nm} e^{-if}) \sin \frac{1}{2} \phi_{mn}, \\ \phi_{mn} &= 2(t - t_0) \gamma H_{rf} |\langle n | I_x | m \rangle|, \hat{1} = \sum_m P_{mm}, \end{aligned} \quad (9)$$

where oscillating magnetic field is parallel to X axis, and H_{rf} , f and $\Omega (= \Omega_{mn} \equiv (E_m - E_n)/\hbar)$ - its amplitude, phase and frequency, and $\hat{1}$ - unit operator in space $\Gamma_{7/2}$. A case when the field is parallel to Y axis results in replacing f by $f + \frac{1}{2}\pi$ in (9).

Let us consider the realization of logic gates on the spin-7/2 states in order of increasing their complexity.

The CCNOT gate requires one single frequency pulse. For example, the gate $CCNOT_{Q,R \rightarrow S}$ is realized using pulse with frequency Ω_{67} and with rotation angle π . According to (9) the evolution operator at such conditions has the following form

$$V_X(\pi_{67}, 0) = \hat{1} - (P_{77} + P_{66}) + i(P_{67} + P_{76}). \quad (10)$$

Taking into account the above mentioned isomorphism one can see that the following equality takes place:

$$P_{67} + P_{76} = |6\rangle \langle 7| + |7\rangle \langle 6| = |110\rangle \langle 111| + |111\rangle \langle 110|. \quad (11)$$

It means that the matrix of evolution operator $V_X(\pi_{67}, 0)$ is equal to matrix of the gate $CCNOT_{Q,R \rightarrow S}$ (Eq. (5)):

$$V_X(\pi_{67}, 0) = CCNOT_{Q,R \rightarrow S} \quad (12)$$

up to the phase factor i for non diagonal elements. For other two gates one has

$$\begin{aligned} V_X(\pi_{75}, 0) &= CCNOT_{Q,S \rightarrow R}, \\ V_X(\pi_{73}, 0) &= CCNOT_{R,S \rightarrow Q}. \end{aligned} \quad (13)$$

It is necessary to point out that in comparison with transition Ω_{67} , the transitions Ω_{57} and Ω_{37} between the states χ_M are forbidden and become non zero in the first order of parameter ω_Q/ω_0 . To get the π rotation in these cases longer pulses or stronger RF field are necessary. However, numerical calculations show, that when ω_Q and ω_0 are of the same order of magnitude, the expressions for rotation angles also have the matrix elements of the same orders.

The CNOT gate requires one double frequency pulse, the evolution operator of which is a product of two operators:

$$\begin{aligned} V_X(\pi_{23}, 0)V_X(\pi_{67}, 0) &= CNOT_{R \rightarrow S}, \\ V_X(\pi_{13}, 0)V_X(\pi_{57}, 0) &= CNOT_{S \rightarrow R}, \\ V_X(\pi_{45}, 0)V_X(\pi_{67}, 0) &= CNOT_{Q \rightarrow S}, \\ V_X(\pi_{15}, 0)V_X(\pi_{37}, 0) &= CNOT_{S \rightarrow Q}, \\ V_X(\pi_{46}, 0)V_X(\pi_{57}, 0) &= CNOT_{Q \rightarrow R}, \\ V_X(\pi_{26}, 0)V_X(\pi_{37}, 0) &= CNOT_{R \rightarrow Q}. \end{aligned} \quad (14)$$

The NOT gate requires one four-frequency pulse, the evolution operator of which is a product of four operators:

$$\begin{aligned} V_X(\pi_{04}, 0)V_X(\pi_{15}, 0)V_X(\pi_{26}, 0)V_X(\pi_{37}, 0) &= NOT_Q, \\ V_X(\pi_{02}, 0)V_X(\pi_{13}, 0)V_X(\pi_{46}, 0)V_X(\pi_{57}, 0) &= NOT_R, \\ V_X(\pi_{01}, 0)V_X(\pi_{23}, 0)V_X(\pi_{45}, 0)V_X(\pi_{67}, 0) &= NOT_S. \end{aligned} \quad (15)$$

The physical realizations of gates, expressed in Eq. (12)-(15), in comparison with adopted in quantum information notation have additional phase factor i for non diagonal elements. It should be taken into account later, when these gates will be used for constructing complex algorithms.

Above for simplicity specific values of parameters ϕ and f have been used in evolution operators. The expressions (12)-(15) for CCNOT, CNOT, NOT can be easily generalized to get expressions for CCUT, CUT, UT. For example, if one uses Eq. (9) with arbitrary parameters ϕ and f , then (12) gives the expression for CCUT. The corresponding calculations are straightforward but rather complicated, and would hide the main idea of the paper.

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